Perspective

Research Challenges in Process Systems Engineering

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Introduction

Companies must design and operate chemical processes effectively and efficiently so they may survive in today's highly competitive world. Providing the methods, tools and people that allow industry to meet its needs by tying science to engineering is a compelling aspect of Process Systems Engineering (PSE). Despite the importance of the PSE, the scope and research of this area are often not well understood. One of the major reasons is that chemical engineering has evolved over the past five decades from being an engineering discipline rooted in the concept of unit operations to one based on engineering science and mathematics, and most recently to one with increasing ties to the natural sciences. This very significant change in emphasis has created a gap between the science-based and the systems-based research in chemical engineering. We argue here that this gap might be closed in two ways: first, by broadening the definition of PSE through the introduction of the concept of the "chemical supply chain;" second, by gaining a better appreciation of the intellectual research challenges in this area. We address the latter issue by discussing the nature and major accomplishments of the PSE area and outlining emerging research directions.

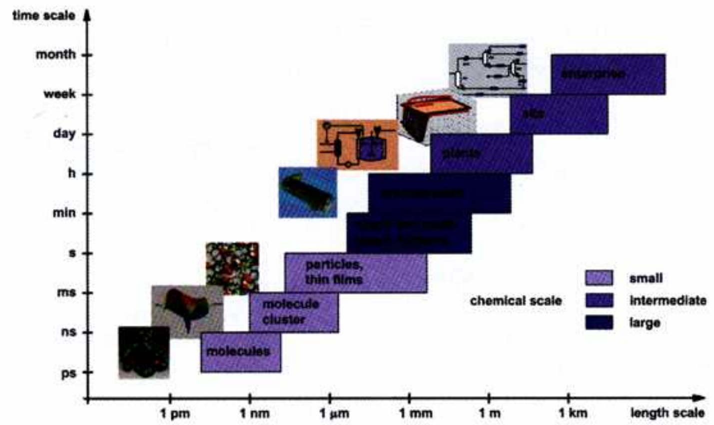

Figure 1. Chemical supply chain.

Broadening the scope of PSE

As explained in the box at the end of this article, PSE is a relatively young area in chemical engineering. PSE is about 35 years old; its progress is closely tied with developments in computing (Edgar et al., 1999).

PSE is concerned with the understanding and development of systematic procedures for the design and operation of chemical process systems, ranging from microsystems to industrial-scale continuous and batch processes. While this definition is adequate, we broaden our definition of PSE by making use of the concept of the *chemical supply chain* shown in Figure 1. The supply chain starts with the set of chemicals that industry must synthesize and characterize at the molecular level. Subsequent steps aggregate these molecules into clusters, particles, and films—as single and multiphase systems that finally take the form of macroscopic mixtures. Transitioning from chemistry to engineering, we move to the design and analysis of the production units, which are integrated into a chemical process that in turn becomes part of a site with multiple processes. Finally, this site is part of the commercial enterprise driven by business considerations.

We now offer the following broader definition of the PSE area:

Process Systems Engineering is concerned with the improvement of decision-making processes for the creation and operation of the chemical supply chain. It deals with the discovery, design, manufacture, and distribution of chemical products in the context of many conflicting goals.

This definition, which relies on the concept of the chemical supply chain, ties fundamental scientific discoveries at the molecular or microscopic level with strategies and logistics for manufacturing and production planning. Furthermore, this definition directly ties to industrial needs from R&D to product distribution. The major goal is to improve all these activities by systematic decision-making, which has both practical and theoretical implications.

From a practical point of view, the implication of the above definition in terms of the chemical supply chain is to provide knowledge and tools to support both the "value preservation" (e.g., large-scale commodity chemicals) and the "value growth" (e.g., specialty chemicals, biotechnology, and pharmaceutical products) industries. The goal is to ensure that both types of industries remain competitive and economically viable. The "value preservation" industry must reduce costs, operate efficiently, and continuously improve product quality, traditional concerns in PSE. These concerns lie largely in the middle and upper part of Figure 1. The "value growth" industry must discover new products and be agile and fast to market, concerns PSEis only now beginning to address. These concerns lie both in the lower and higher ends of Figure 1.

Nature of PSE research and accomplishments

While largely driven by industrial needs, it is important to understand that PSEresearch also deals with fundamental theoretical issues. Science views as its intellectual challenge the discovery and rationalization of natural phenomena. In contrast, the intellectual challenges for the PSE area are the discovery of concepts and models for the prediction of performance and for decision-making for an engineered system. Science strives to unravel the underlying mechanisms that explain the behavior of a system. Again, in contrast, PSE research strives to create representations and models to generate reasonable alternatives, and then select from among them a solution that meets constraints and ideally optimizes an objective. In science-based areas, with few exceptions (e.g. astrophysics), experiments are a key step for validating a hypothesis. The PSE area can also have validation through experiments for physically existing systems, but, in most cases, PSE has only "virtual" systems in the form of models (e.g., in the conceptual phase of a design). One can test the models, ideally by proving and disproving theorems about them, but, more often, one can only prove mathematically some useful properties or empirically demonstrate that the proposed model works for a set of example problems.

Computational efficiency is also an intellectual challenge in the PSE area. While areas of science such as molecular simulation, bioinformatics, and computational-fluid dynamics share this concern, most areas of science do not. Solution efficiency arises in the PSEarea for two reasons. First, the selection problems that we generate (decision-making as opposed to analysis) are often NP-hard (see Garey and Johnson, 1978), which means that in the worst case the computation increases exponentially with problem size. Therefore, we can easily challenge and will continue to challenge our best computers for reasonably sized engineering problems. Second, we may be using our models in a real-time environment in which computations, to be of use, must be completed within tight time windows.

From the above discussion, we note that the PSEarea is closely tied to mathematics, operations research, and computer science. It is a "human-made" science, which deals with objects created by humans such as a chemical process, a model of a physical system, or an algorithm. These objects are not found in nature. As in mathematics, models may not have closed form solutions, which in fact is typically the case. As in operations research, developing good problem representation for the alternatives is central to the development of PSE models. Lastly, as in computer science, the model typically manifests itself as a piece of software, often a very complex one.

Developing novel representations and models that capture nontrivial features, as well as developing computationally efficient solution methods and software tools that provide new capabilities, are all considered to be original contributions in PSE. Lacking space, we list in Table 1 only a few of the major accomplishments that have occurred in the past three decades in this area.

Future challenges

Having provided a broader perspective of PSE in terms of the chemical supply chain and having discussed the nature of the research in this area, we note the following major drivers for future research in the PSE area (Grossmann and Siirola, 2000). Globalization of trade and competition will lead to low margins, increasing the competitive importance of technological advantage and efficient operation. Increased investor pressure will create demands for improved earnings performance from both commodity and specialty product manufacture. Internet and electronic commerce will require lightening-fast decision-making, shifting the power to the customer and requiring flexible manufacture for custom specification within a tight schedule. New environmental pressures will increase, including carbon dioxide emission considerations and restrictive waste disposal. New chemistries will require new processes that can handle changing feedstock availability, less gas condensate, temporarily more naphtha and coal, and greater ultimate use of renewable and recovered feedstocks. All of these drivers will demand new discoveries and developments in PSE that should cover all length and time scales of the subsystems involved in Figure 1.

Based on these drivers, the following are some of the likely topics that will emerge as major challenges in the PSE area over the next decade.

Process and Product Design. In order to move towards the molecular level, traditional process design will be expanded to include product design, with particular emphasis on design of new molecules. The major difference here will be the need to develop predictive capabilities for properties of compounds and mixtures of compounds, ranging from fluids to structured materials, and the systematic generation of alternatives in order to apply methodologies developed previously for structural decisions in process design (e.g., hierarchical decomposition, superstructure optimization). Within the commodity chemicals industry, a major challenge that will be addressed is process intensification—e.g., by discovering novel unit operations or microsystems that integrate several functions and that can potentially reduce the cost and complexity of process systems. Another major challenge that will remain is the design of sustainable and environmentally benign processes. Areas that are likely to receive increased attention due to the growth in new industries include molecular design, synthesis of microchips and bioprocess systems, and design and analysis of metabolic networks. This trend may in principle give rise to design problems that have not received much attention (e.g., separation of very dilute systems).

Process Control. The considerable developments that have taken place in process control will be aimed towards a tighter integration between design and control, and expanded towards new applications such as bioprocesses and biomedical devices that are likely to require the use of nonlinear control concepts. For the commodity chemicals industry, there will be increased need for synthesizing plantwide control systems and effective application of plantwide model predictive control in order to provide a seamless integration with business planning and supply chain management. Another trend will be to integrate discrete events and safety functions fully in the regulatory process control. One promising avenue to achieve this goal is new developments in hybrid systems, an area that is concerned with simulation and optimization problems involving continuous and discrete states in dynamic systems. At the other extreme, the rapid improvement of sensors, that may themselves be miniature processes, will be coupled with powerful miniature computers and will remake what we can sense and react to locally.

R&D and Process Operations. The area of process operations, which has a shorter history than process design and control, will expand upstream to R&D and downstream to logistics and product distribution activities. To support the expansion to R&D, optimal planning and scheduling for new product development will receive increased attention to coordinate better product discovery, process development, and plant design in the agrochemical and pharmaceutical industries. For downstream applications, areas that will receive increased attention at the business level include planning of process networks, supply chain optimization, real-time scheduling, and inventory control. At the plant level, areas of interest will include process verification and synthesis of operating procedures, both of which impact the safety of plant operations. Applications will be aimed at large-scale continuous processes, commonly found in commodities, and to small-scale batch processes, commonly found in specialties.

Modeling. In PSE, modeling is of paramount importance. In order to be able to model all the various aspects involved in the chemical supply chain of Figure 1, more flexible modeling environments will be required that can accommodate a greater variety of models, ranging from molecular level to macroscopic systems. This implies being able to pose from the simpler algebraic to the more complex partial differential algebraic models, both in pure equation form and with mixed procedures. Furthermore, for discrete/continuous optimization, the combination of quantitative and qualitative models expressed through equations and logic will be increasingly important. The capability of automating problem formulation through higher level physical descriptions should also be an area of potentially great impact.

Table 1. Significant Accomplishments in PSE in the Past Three Decades

Process Design	Process Operations
Synthesis of energy recovery networks	Scheduling of process networks
Synthesis of distillation systems (azeotropic)	Multiperiod planning and optimization
Synthesis of reactor networks	Data reconciliation
Hierarchical decomposition flowsheets	Real-time optimization
Superstructure optimization	Flexibility measures
Design multiproduct batch plants	Fault diagnosis
Process Control	**Supporting Tools**
Model predictive control	Sequential modular simulation
Controllability measures	Equation based process simulation
Robust control	AI/Expert systems
Nonlinear control	Large-scale nonlinear programming (NLP)
Statistical Process Control	Optimization of differential algebraic equations (DAEs)
Process monitoring	Mixed-integer nonlinear programming (MINLP)
Thermodynamics-based control	Global optimization

Integration. The integration of several parts of the chemical supply chain in Figure 1 will give rise to a number of challenges—such as multiscale modeling ranging from molecular dynamics, to integration of planning, to scheduling and control (internet based)—and the integration of measurements, control, and information systems. The concept of life-cycle modeling will also be expanded as a way of integrating all the major phases that a product goes through, from discovery through process development, design, manufacturing, distribution, and disposal.

Supporting Methods and Tools. To make progress in most of the above areas will require a number of new supporting methods and tools that currently are not available. These include large-scale differential-algebraic methods for simulating systems at multiple scales (e.g., fluid mechanics and molecular dynamics), a capability that is still at a very early stage. There is also need for methods for simulating and optimizing under uncertainty, a capability that is also in its infancy. Another important capability will be advanced optimization tools that can handle mixed-integer, discrete-logic, and quantitative-qualitative equations that may be algebraic, dynamic, and/or distributed to model synthesis and planning and scheduling problems more effectively. There is need of improved methods to determine global optima for arbitrary functions and improved real-time optimization methods to handle extremely large nonlinear models involving millions of variables. Improved tools for accommodating heuristic reasoning and hierarchical computations for conceptual design will also be required. Information modeling tools will become increasingly important for supporting integration problems and for problem solving by large and globally distributed teams. The other application of information modeling and data mining will be in the area of bioinformatics.

Advances in computing will help to realize some of the supporting tools described above. While parallel computing is likely to continue to have an impact in specialized applications, it is also likely that it will rely less on specialized users since many parallel functions are likely to become automated through advanced software and distributed computing. We can continue to except a higher number of cycles and larger memories, which will help in addressing larger problems. A new capability, whose impact is still somewhat difficult to predict, is wireless computing. One area that is likely to benefit is in the integration of measurements, control and information systems. Wireless computing may also create new needs for effectively supporting teamwork by diverse and distributed specialists. Finally, there are new potential applications from software and internet-based computing. The demand for software development may increase as chemical engineering moves to new areas in which there are no standard software packages. Internet-based computing offers the exciting possibility of more readily sharing new software developments directly from the developers and of integrating these more rapidly with existing software packages.

In summary, it is clear that there are plenty of intellectually challenging problems in PSE that are awaiting solutions from individuals with creative minds. We believe that by broadening the definition of Process Systems Engineering, as we have outlined with the concept of the chemical supply chain, we can reduce the gap between science-based and systems-based research. This will be essential if chemical engineering is to remain a vibrant profession that is of relevance to industry.

Literature cited

Edgar T. F., D. A. Dixon, and G. V. Reklaitis, "Vision 2020: Computational Needs of the Chemical Industry," *Impact of Advances in Computing and Communication Technologies on Chemical Science and Technology*, National Research Council, National Academic Press, Washington, DC (1999).

Garey, M. R., and D. S. Johnson, *Computers and Intractability: A Guide to the Theory of NP-Completeness*, W. H. Freeman and Company, New York (1978).

Grossmann, I. E., and J. J. Siirola, “Process Systems Engineering,” *Challenges for the Chemical Sciences in the 21st Century*, R. Breslow and R. Brown, eds., NRCReport in press.

Marquardt, W., L. Von Wedel, and B. Bayer, “Perspectives on Lifecycle Process Modeling,” AIChE Symposium Series, 96(323), 192 (2000).

Westerberg, A. W., National Research Council Committee on Chemical Engineering Frontiers, Head of Panel on Computer Assisted Process and Control Engineering (1984–1988).

Process Systems Engineering is a relatively young area in chemical engineering. The first time that this term was used was in a Special Volume of the AIChE Symposium Series in 1961. However, it was not until 1982 when the first international symposium on this topic took place in Kyoto, Japan, that the term PSE started to become widely accepted. The first textbook in the area was *Strategy of Process Engineering* by Dale F. Rudd and Charles C. Watson, by Wiley (1968). The Computing and Systems Technology (CAST) Division, Area 10 of AIChE, was founded in 1977 and currently has about 1,200 members. CAST has four sections: Process Design, Process Control, Process Operations and Applied Mathematics. The first journal devoted to PSE was *Computers and Chemical Engineering*, which appeared in 1977, with the late Richard Hughes being the editor. The current coeditors are G. V. Reklaitis, Manfred Morari, and Jack Ponton. The Foundations of Computer-Aided Process Design (FOCAPD) conference held in Henniker in 1980 was one of the first meetings in a series on that topic in the PSE area. It is now accompanied by the successful series on Control (CPC), Operations (FOCAPO), and the worldwide series entitled *Process Systems Engineering*. The CACHE Corporation (Computer Aids for Chemical Engineering), which organizes these conferences, was initially launched by academics in 1970, motivated by the introduction of process simulation in the chemical engineering curriculum. There are currently about 80 academics in the PSE area in the U.S., and a list of these faculty can be found in **http://cepac.cheme.cmu.edu/pse1.html**. A very large fraction of the faculty in the PSE area can be traced back to Professor Roger Sargent from Imperial College, one of the pioneers in the area. PSE is an active area of research in many other countries, particularly in the U.K, several other European countries, Japan, Korea, and China. Since 1992, Europe hosts the annual ESCAPE meeting (European Symposium of Computer Aided Process Engineering). Each produces proceedings—e.g., see *Comput. Chem. Eng.*, Vol. 21 Supplement (1997) for the Proceedings of the joint PSE ’97/ESCAPE 7 meeting held in 1997.